Probing Kitaev Models on Small Lattices

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We address the following important question: how to distinguish Kitaev models experimentally realized on small lattices from other non-topological interacting spin models. Based on symmetry arguments and exact diagonalization, we show that a particularly characteristic pattern of spin-spin correlations survives despite finite size, open boundary and thermal effects. The pattern is robust against small residual perturbing interactions and can be utilized to distinguish the Kitaev interactions from other interactions such as antiferromagnetic Heisenberg interactions. The effect of external magnetic field is also considered and found to be not critical.

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A great deal of interest [1, 2, 3] has recently focused on the possible realization of exotic anyonic quasi-particle statistics in two-dimensional interacting topological systems. Much of this interest arises from the intrinsic fundamental significance of anyons, which are neither fermions nor bosons, and are thus theoretically allowed only in two dimensions where particle exchange is characterized by the braid group rather than the permutation group (as in ordinary three dimensional systems). The possibility of carrying out fault-tolerant topological quantum computation [1, 2, 3, 4] using anyonic braiding is another key reason for the current interest in the subject.

Broadly speaking, there are two alternative and complementary routes which have been pursued in the literature for the physical realization of the topological phase and anyonic quasi-particles. One route [1] is studying physically occurring quantum states in nature which are believed (or perhaps conjectured) to be anyonic in character because their low-energy properties are thought to be well-described by some model topological quantum field theory. The prime example of such a situation is the 5/2 fractional quantum Hall state [5] which is widely considered to belong to the $(SU_2)_2$ conformal field theory [1]. A great deal of experimental [6] and theoretical [7] work is currently being pursued all over the world with the goal of realizing the fractional quantum Hall topological qubit using the non-Abelian anyonic quasi-particle braiding statistics [1]. Closely related to the 5/2 topological fractional quantum Hall state is the chiral p-wave superconducting state [8] in $SrRuO_3$ or cold atoms where anyonic Majorana particles may exist. The second route to the realization of the topological phase, pioneered by Kitaev [2, 3] and the subject matter of our work, involves the explicit construction of model spin Hamiltonians which, by design, have topological ground states with Abelian or non-Abelian anyonic quasi-particle excitations. In addition to the Kitaev model, topological matter in this category of model Hamiltonian systems includes the Levin-Wen model [9]. We note the interesting (and somewhat ironic) dichotomy between the two classes of topological matter discussed above: in the first category, the physical systems (e.g. the 5/2 quantum Hall state) exist in nature, but may not be topological, whereas in the second category the model Hamiltonians are, by design, topological, but may not exist in nature!

In this letter, we consider the important issue of the extent to which the topological character of the Kitaev model can be preserved in a finite size system (e.g. a few plaquettes only), which could possibly be physically implemented in an atomic system such as an ion trap lattice with 20-30 ions or a cold atom (or molecular) optical lattice with suitable interactions. We do not discuss the logistical question of how to construct such a lattice, which has much been discussed in the recent literature [10]. Our focus here is on the deep and fundamental question of which characteristic properties of the thermodynamic Kitaev model could be manifested in a finite size lattice of only a few plaquettes. We find, rather surprisingly, that a few plaquettes may be enough to preserve several characteristic features of the Kitaev model. An important possible application of our results could be the development of techniques to check whether a particular finite size atomic (or ionic or molecular) system is likely to manifest topological behavior. Given the great recent success of atomic systems as emulators of well-known strongly correlated model Hamiltonians (e.g. the Bose-Hubbard model and the fermionic Hubbard model), it seems likely that a small finite size Kitaev model made of ion traps or polar molecules could lead to the emulation of a topological phase in the laboratory. Our theoretical results, establishing the impressive robustness of topological matter, arising from the large number of nontrivial independent conserved operators in the model and quantitatively verified by explicit exact diagonalizaiton calculations, apply to both the Kitaev honeycomb lattice and the toric code. In addition to the finite size behavior of the Kitaev model, we also study the robustness of such small systems to possible perturbing interactions and external magnetic fields, establishing quantitative criteria for the observation of the characteristic thermodynamic Kitaev model features in realistic small atomic systems.

In this work, we focus on the measurements of local objects such as spin-spin correlations and magnetization in an open boundary system. We are motivated by the existence of a large set of local conserved quantities in the Kitaev models [2, 3]. Based on symmetry arguments, we are able to conclude that the local conserved quantities impose very strict constraints on spin-spin correlations [11], and an extremely characteristic pattern emerges in the spatial distribution of spin-spin correlations. More interestingly, this pattern is protected against small size, open boundary, and thermal effects. It is also robust against small perturbing interactions that may be present in realistic experimental setups. Our main results are summarized in Fig.2 where the characteristic ordered emergent correlation pattern of the Kitaev model are compared with the messy results of the anisotropic Heisenberg model shown in Fig.3.

We first study the Kitaev model [3] on a honeycomb lattice sketched in the top left panel of Fig.2,

$$H = \sum_{\alpha=x,y,z} \sum_{\alpha-bonds} J_\alpha \sigma_b^\alpha \sigma_w^\alpha, \tag{1}$$

where the subscripts b and w denote the two end sites(black or white) of nearest-neighbor bonds and σ's are the Pauli matrices. This model has two phases [3]. The gapped phase has Abelian anyons as excitations, whereas the gapless one supports non-Abelian anyonic excitations in the presence of an external magnetic field. In this work, we study the case of $J_x = 0.4, J_y = 0.4$ and $J_z = 1.0$ which is gapped. Our symmetry argument holds for both gapped and gapless phases.

For each plaquette, there is one conserved quantity. For instance, for the plaquette enclosed by sites 1-6, the operator $W_p = \sigma_1^y \sigma_2^z \sigma_3^x \sigma_4^y \sigma_5^z \sigma_6^x$ is conserved [3]. These conserved quantities have profound implications for the physics of the Kitaev model [3, 11, 12, 13]. For spin-spin correlations, it is always possible to find a conserved quantity that flips one spin without changing the others, unless the following two conditions are both satisfied [11]:

- The two spins are nearest neighbors;
- Their components agree with the bond direction.

The spin-spin interaction terms in Eq.(1) satisfy the above two conditions. If the conservation law applies, the correlation functions vanish identically unless the above conditions are both satisfied.

However, for the open boundary case, the boundary terms, such as $W = \sigma_1^z \sigma_2^y$ in the 16-site lattice of Fig.2, may not commute with each other. For instance, $[\sigma_1^z \sigma_2^y, H] = [\sigma_2^x \sigma_3^z \sigma_7^z, H] = 0$ but $[\sigma_1^z \sigma_2^y, \sigma_2^x \sigma_3^z \sigma_7^z] \neq 0$. Therefore, in a pure ground state, some of the symmetries involving the boundary spins might be broken, and consequently the spin-spin correlation functions involving the boundary spins can have finite values. In the 16-site lattice of Fig.2, only the 4-th and 10-th sites are not on the boundary and the remaining 14 sites are all boundary sites. In Fig.1, we plot the correlation functions in a typical pure ground state of the 16-site Kitaev model with parameters $J_x = 0.3$, $J_y = 0.4$ and $J_z = 1.0$. As expected, finite correlations are found between the boundary spins. Furthermore, the ground state is 16-fold degenerate. This can be understood based on the exact mapping introduced in Ref. [11, 14]. Sites 2, 7, 12, 16 have dangling Majorana fermions, each of which contributes a factor of $\sqrt{2}$ to the ground state degeneracy. Also, each horizontal row of the z-bonds has a Z_2 degree of freedom. Combining all these contributions, we obtain the degeneracy $(\sqrt{2})^4 \times 2^2 = 16$.

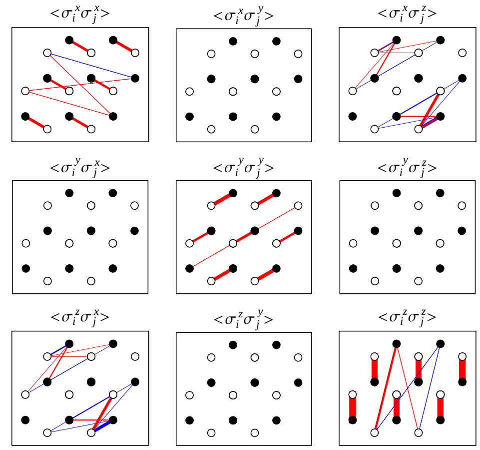

FIG. 1: Spin-spin correlation functions of the 16-site Kitaev model in a pure ground state. The coupling strengths are $J_x = 0.3, J_y = 0.4$ and $J_z = 1.0$. Red(Blue) bond denotes negative(positive) correlation. Bond thickness is proportional to the magnitude of the correlation. Empty bonds denote zero correlations.

Since the ground state is degenerate, different pure ground state wavefunctions lead to different spin-spin correlation functions. Therefore, it is important to control the experimental realization of the ground state. One interesting and simple situation is the thermal equilibrium state instead of a pure state. For a thermal equilibrium state at zero temperature, the density matrix is $\rho \propto \sum_{|g.s.\rangle} |g.s.\rangle\langle g.s.|$, where the summation is over all degenerate ground states $\{|g.s.\rangle\}$. In this symmetric mixed state, the broken symmetries are restored, and one would expect correlation functions to vanish unless the two conditions are satisfied. This can be easily seen from the exact diagonalization results plotted in Fig.2. We thus obtain our main result. The spin-spin correlation functions of the Kitaev model on the honeycomb lattice are extremely short ranged and anisotropic. As a comparison, we plot the correlation functions of the anisotropic Heisenberg model on the same 16-site lattice in Fig.3. In this case, the correlation functions are all over the real space and dramatically different from the case of Kitaev model in Fig.2.

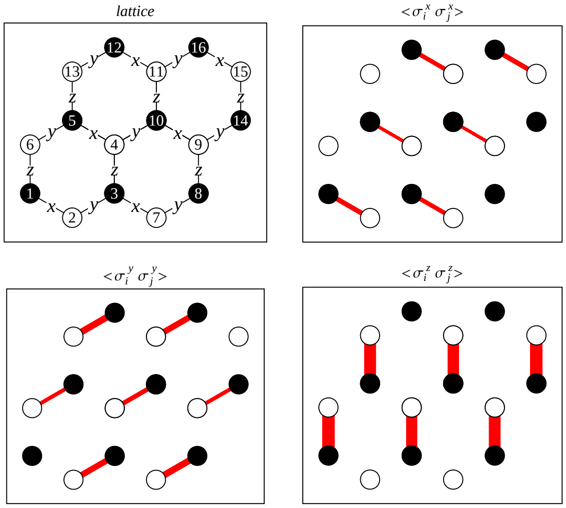

FIG. 2: Top-left: Honeycomb lattice of 16 sites and three types of bonds. Others: spin-spin correlations in the low temperature thermal equilibrium state. All other components such as $\langle\sigma^x\sigma^y\rangle$ vanish identically.

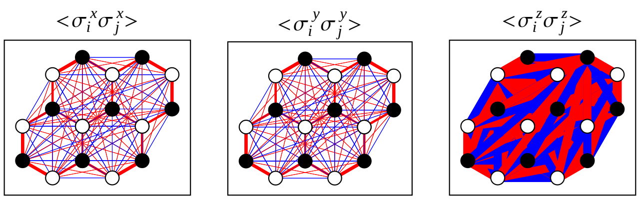

FIG. 3: Spin-spin correlations for the anisotropic Heisenberg model $H = \sum_{<bw>}\sum_\alpha J_\alpha \sigma_b^\alpha \sigma_w^\alpha$ with parameters $J_x = 0.3$, $J_y = 0.4$ and $J_z = 1.0$. This is dramatically different from the case of Fig.2 of Kitaev model.

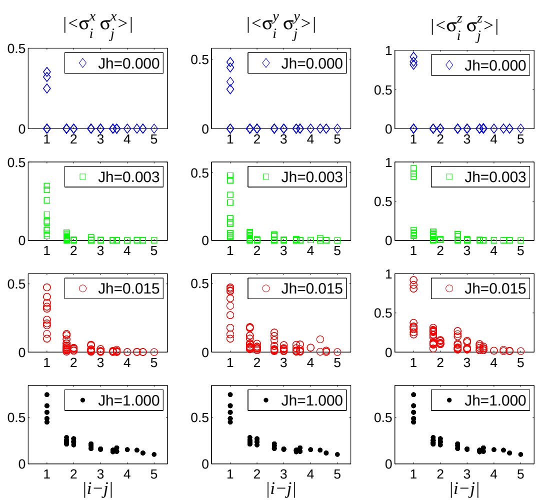

FIG. 4: Spin-spin correlation functions on a lattice of 16 sites. Top three panels are pure Kitaev model and the Bottom three panels are pure antiferromagnetic Heisenberg model. Middle six panels are Kitaev model with residue Heisenberg interactions. The parameters for Kitaev model are $J_x = 0.3$, $J_y = 0.4$, $J_z = 1.0$.

Because unwanted perturbing interactions are inevitable in any experimental realization, it is necessary to study their effects. In particular, we consider the uniform antiferromagnetic Heisenberg interaction $H_{res} = J_h \sum_{<bw>}\sum_\alpha \sigma_b^\alpha \sigma_w^\alpha$. Although this perturbation destroys the local conserved quantities, the pattern in Fig.2 survives when the residual interaction is a few percent of the coupling strength J_x, J_y, J_z. In Fig.4, we plot the calculated correlations in the presence of antiferromagnetic perturbation as functions of the distance between two spins. In the top panels, we plot the results of a pure Kitaev model. One can only find finite correlations for some of the nearest neighboring bonds, as we discussed previously. As we increase the perturbation to $J_h = 0.003$, which is 1% of J_x, small correlations start to develop between next-nearest-neighbors and next-next-nearest neighbors. Nevertheless, the dimerization along z-bonds is still very strong, *i.e.*, the difference between strong and weak $\langle\sigma^z\sigma^z\rangle$ correlations remains evident. As the perturbation further increases to 5% of J_x ($J_h = 0.015$), more long range correlations emerge and reach as high as about 30% of the strongest correlations of the nearest-neighbor bonds. However, it still has a much shorter tail than the pure Heisenberg model, which is shown in the bottom panels. Furthermore, the difference between strong and weak $\langle\sigma^z\sigma^z\rangle$ correlations is still visible. Therefore, we conclude that it is necessary to control any residual interactions within a few percent of the Kitaev coupling strength to successfully observe the characteristic Kitaev pattern depicted in Fig.2.

We now turn to another important effect, namely the effect of an external magnetic field. When an external magnetic field is applied, the conserved quantities defined on plaquettes are no longer good quantum numbers. However, other conserved quantities defined on the zig-zag chains might survive. When the field is along the z-direction, the products of σ^z on the horizontal zig-zag chains, *e.g.* $\sigma_1^z\sigma_2^z\sigma_3^z\sigma_7^z\sigma_8^z$, still commute with the full Hamiltonian and with each other. Consequently, the correlations between two spin components along x or y directions can have finite values only if they belong to the same horizontal zig-zag chains, as seen in the first two panels of Fig.5. Longer range correlations are developed in the z-components. As long as B is small compared with J_z, z-bonds are still dominated by singlets formed between two end spins. Overall, the characteristic pattern of Fig.2 is clearly visible in Fig.5. On sites $2, 7, 12, 16$, where dangling Majorana fermions exist when $B = 0$, sizeable spin moment is induced along the field direction, as plotted in the third panel of Fig.5. Significant magnetization along the field direction is thus observed even for a small magnetic field, as shown in Fig.6. This is opposite to the case of anisotropic Heisenberg model, where a spin gap prevents the magnetization of spins at low temperature.

At finite temperature, excited states will also contribute to the correlation functions. Fortunately, the

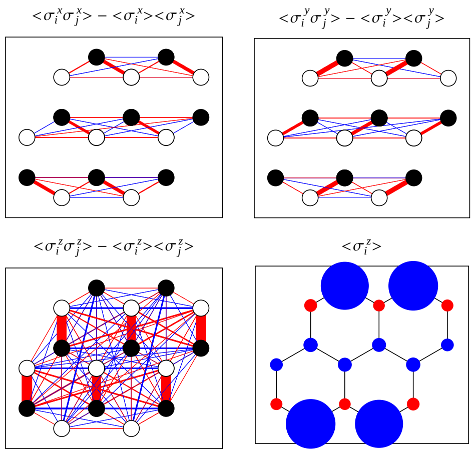

FIG. 5: Spin-spin correlations and spin moment in the low temperature thermal equilibrium state when a uniform magnetic field $B_z = 0.1$ along the z direction is applied. In the right-bottom panel, red(blue) denotes negative(positive) moment. The size of dot denotes the magnitude of spin moment. $\langle \sigma_2^z \rangle = 0.78$.

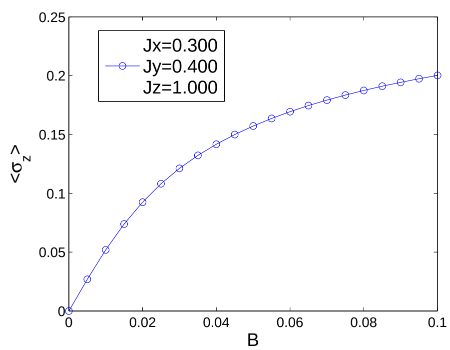

FIG. 6: Magnetization $\sum_i \langle \sigma_i^z \rangle / 16$ in Kitaev model as a function of uniform external magnetic field B_z along the z direction.

symmetry argument holds not only for the ground state but also for excited states. The pattern of Fig.2 is thus protected by the local symmetries, and thermal fluctuations have no effect on it.

Finally, we also study an equivalence of the Kitaev toric code [15, 16]. The model is defined on a square lattice,

$$H_{toric} = \sum_{\vec{r}} J \sigma_{\vec{r}}^x \sigma_{\vec{r}+\hat{e}_x}^y \sigma_{\vec{r}+\hat{e}_x+\hat{e}_y}^x \sigma_{\vec{r}+\hat{e}_y}^y \qquad (2)$$

where $\vec{r}$ is the lattice point of square lattice spanned by $\hat{e}_x$ and $\hat{e}_y$. This model proposed by Wen[15] was shown to be equivalent[16] to the toric code of Kitaev[2]. The terms in Eq.(2) commute with each other and form a large set of local conserved quantities. It is thus possible to apply similar symmetry arguments and obtain similar constraints on spin-spin correlation functions. However, in this model, the symmetry argument does not apply

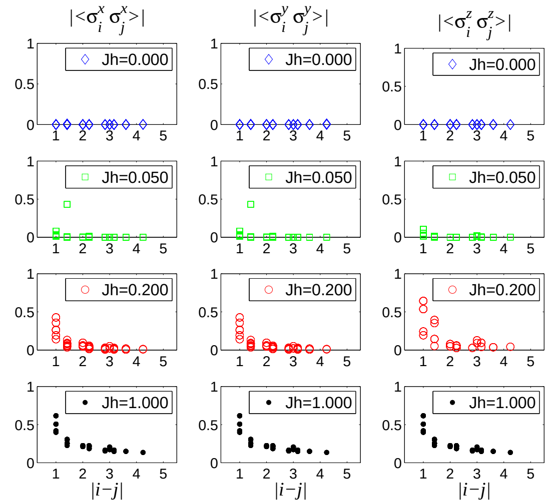

FIG. 7: Correlations in toric code model of Eq.(2). Top three panels are pure toric code model. The second and third rows are toric mode with uniform antiferromagnetic Heisenberg interactions. The last row is pure Heisenberg model on square lattice. The coupling strength of toric code is $J = 1$.

to some bonds near the four corners of the square lattice. Nevertheless, as we can see in the first row of Fig.7, spin-spin correlations vanish or are negligibly small. As a perturbing Heisenberg interaction is introduced, small correlations start to emerge. When $J_h = 0.2J$, the spin-spin correlations are already dominated by the perturbing interactions, as shown in the third and fourth rows in Fig.7. Therefore, we conclude that to observe the toric code on small lattices, one has to limit residual interactions up to a few percent of the coupling strength J.

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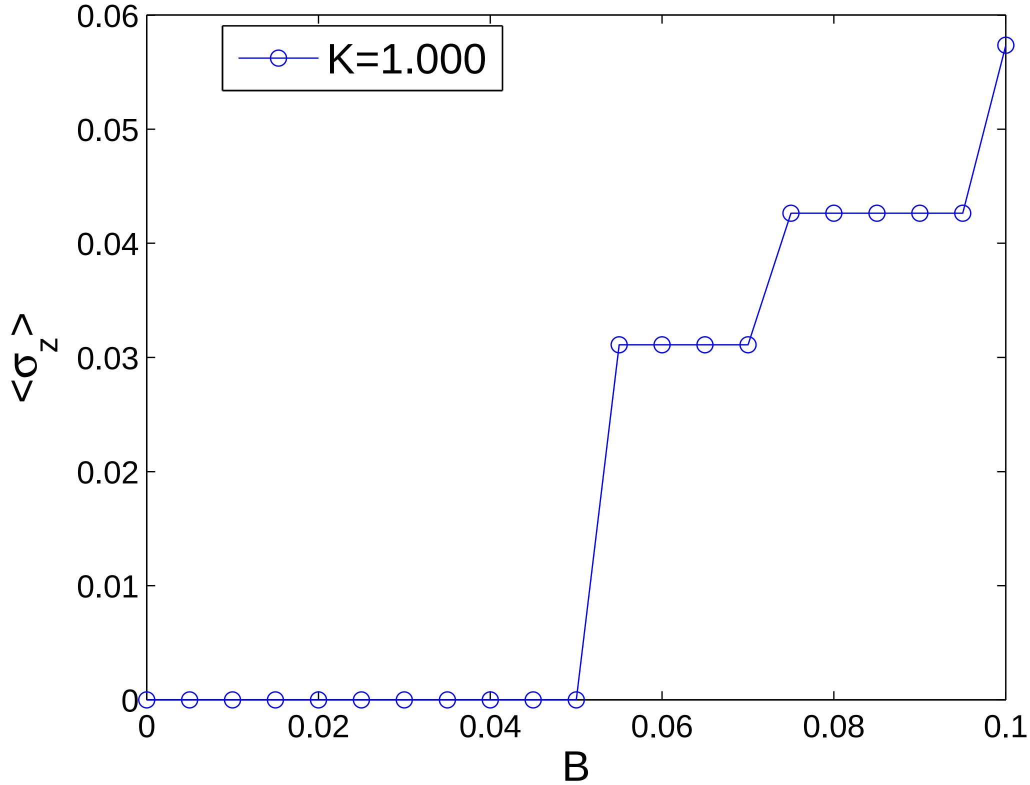

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